ABSTRACT

A method for executing calculation of the Hartree-Fock method in a molecular orbital method by a distributed memory parallel computing system includes the steps of: using a computer cluster made up of a plurality of computers; dividing a density matrix into multiple density submatrixes and distributing them to the individual computers and storing therein; and executing calculation processes such as two-electron integration or the like relating to density submatrixes in each computer while sequentially transferring the multiple density submatrixes between the multiple computers.